

⑤ Radial Equation : $V(\vec{r}) = V(r)$

$$-\frac{\hbar^2}{2m} \left[\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + V_{\text{eff}}^{(l)}(r) \right] R_{nl}(r) = E R_{nl}(r)$$

$$\downarrow R = \frac{U(r)}{r} \quad \parallel V_{\text{eff}}^{(l)}(r) = V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} \quad \text{... an effective potential.}$$

$$-\frac{\hbar^2}{2m} \frac{d^2 U}{dr^2} + V_{\text{eff}}^{(l)}(r) U(r) = E U(r)$$

1D Schrödinger eq.

* normalization

• Behavior at $r \rightarrow 0$.

$$1 = \int r^2 dr |R|^2 = \int dr^2 |U|^2$$

We may write $U(r) \sim r^s$ at $r \rightarrow 0$ if it well-behaves.

$$\Rightarrow -\frac{\hbar^2}{2m} s(s-1) r^{s-2} + V(r) r^s + \frac{\hbar^2 l(l+1)}{2m} r^{s-2} = E r^s$$

Leading-order terms

|| assume that
 $r^2 V(r) \rightarrow 0$ as $r \rightarrow 0$.

$$\Rightarrow s(s-1) = \hbar(l+1)$$

$$\therefore s = l+1 \quad \text{or}$$

unphysical!

~~$s = -l$~~

Why? Normalization

$$\int_0^\infty dr r^{-2l} : \text{undefined when } l \geq 1$$

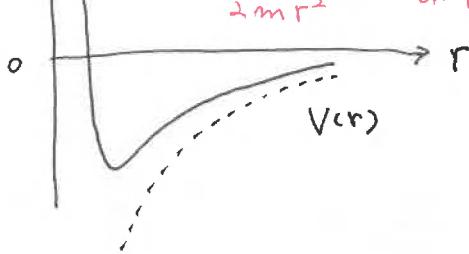
$$\text{if } l=0, R \sim \frac{1}{r}$$

$$\rightarrow \nabla^2 \frac{1}{r} = 4\pi \delta(\vec{r})$$

But the Schrödinger eq.
has no source!

$V_{\text{eff}}(r)$ for $l \neq 0$.

$\frac{\hbar^2 l(l+1)}{2mr^2} \frac{1}{r^2}$: centrifugal BARRIER
on Ang. Mom. barrier.



⑥ Infinite Spherical Well : $V = \begin{cases} 0 & r \leq a \\ \infty & r > a. \end{cases}$

$$-\frac{\hbar^2}{2m} \left(\frac{d^2R}{dr^2} + \frac{2}{r} \frac{dR}{dr} \right) + \frac{l(l+1)}{2mr^2} \hbar^2 R = ER$$

by setting $k = \sqrt{\frac{2mE}{\hbar^2}}$, and $\rho = kr$

$$\rightarrow \frac{d^2R}{d\rho^2} + \frac{2}{\rho} \frac{dR}{d\rho} + \left[1 - \frac{l(l+1)}{\rho^2} \right] R = 0.$$

Sol. $R(\rho) = \begin{cases} j_l(\rho) = (-\rho)^l \left[\frac{1}{\rho} \frac{d}{d\rho} \right]^l \left(\frac{\sin \rho}{\rho} \right) & \text{spherical Bessel fn.} \\ n_l(\rho) = -(-\rho)^l \left[\frac{1}{\rho} \frac{d}{d\rho} \right]^l \left(\frac{\cos \rho}{\rho} \right) & \text{spherical Neumann fn.} \end{cases}$

But, $n_l(\rho) \rightarrow \rho^{l-1}$ as $\rho \rightarrow 0$.

$\therefore R(\rho) \propto j_l(\rho)$

∴ unphysical!

$\rightarrow \sim \rho^l$ as we argued it has to be.

boundary condition

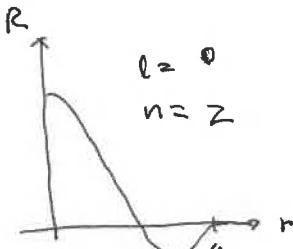
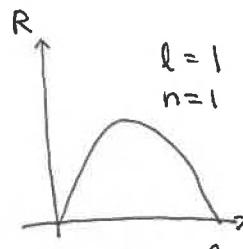
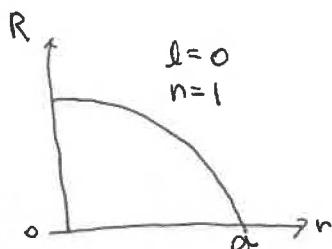
$j_l(ka) = 0 \rightarrow \text{quantization of } E.$

ex. $l=0$: $j_0(ka) = \frac{\sin ka}{ka} = 0$

$$\rightarrow ka = n\pi$$

• $E_{l=0} = \frac{\hbar^2}{2m} \left(\frac{n\pi}{a} \right)^2 \quad \text{if } n = 1, 2, 3, \dots$

ex. $l=1$: $j_1(ka) = \frac{\sin ka}{(ka)^2} - \frac{\cos ka}{ka} \quad \text{needs numerics. to compute } E_{l=1}$



⑦ The Hydrogen Atom.

$$V(\vec{r}) = -\frac{ze^2}{r}$$

One-body problem.

r : relative coordinate.

$m = \mu$: reduced mass

$$= \frac{m_e m_p}{m_e + m_p} \simeq m_e \quad (m_p \gg m_e)$$

$$\Rightarrow \text{radial equation: } \left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{l(l+1)}{2mr^2} \hbar^2 - \frac{ze^2}{r} \right] u = Eu$$

by setting $\rho \equiv kr$ where $K = \sqrt{\frac{2m|E|}{\hbar^2}}$ $\parallel E < 0$.

$$\Rightarrow \frac{d^2u}{d\rho^2} - \frac{l(l+1)}{\rho^2} u + \left(\frac{\rho_0}{\rho} - 1 \right) u = 0$$

$$\text{where } \rho_0 = \sqrt{\frac{2m}{|E|}} \cdot \frac{ze^2}{\hbar} = \sqrt{\frac{2mc^2}{|E|}} \cdot z \alpha$$

($\alpha \equiv e^2/\hbar c \approx 1/137$: fine structure const.)

In the limit of $\rho \rightarrow \infty$,

$$\frac{d^2u}{d\rho^2} - u = 0 \rightarrow u \sim \begin{cases} e^{-\rho} \\ e^{\rho} \end{cases} \text{ unphysical.}$$

so, we can attempt to find a solution in the form of

$$u(\rho) = e^{l+1} e^{-\rho} w(\rho)$$

$$\Rightarrow \rho \frac{d^2w}{d\rho^2} + 2(l+1-\rho) \frac{dw}{d\rho} + [l_0 - 2(l+1)] w(\rho) = 0$$

Try a power-series solution

$$w(\rho) = \sum_{k=0}^{\infty} c_k \rho^k \quad \text{if } c_0 \neq 0,$$

to keep the behavior at $r \rightarrow 0$.



Two-body problem.

$$\rightarrow \sum_{k=2}^{\infty} C_k \cdot k \cdot (k-1) \rho^{k-1} + 2(l+1) \sum_{k=1}^{\infty} C_k \cdot k \cdot \rho^{k-1}$$

$$- 2 \sum_{k=1}^{\infty} C_k \cdot k \cdot \rho^k + [\rho_0 - 2(l+1)] \sum_{k=0}^{\infty} C_k \rho^k = 0$$

$$\rightarrow \sum_{k=1}^{\infty} C_{k+1} (k+1) \cdot k \rho^k + \sum_{k=0}^{\infty} (2k+2) C_{k+1} (k+1) \rho^k$$

$$+ \sum_{k=1}^{\infty} (-2) C_k \cdot k \cdot \rho^k + [\rho_0 - 2(l+1)] \sum_{k=0}^{\infty} C_k \rho^k = 0$$

$$\rightarrow \sum_{k=0}^{\infty} \left[[k(k+1) + 2(l+1)(k+1)] C_{k+1} - [2k+2(l+1) - \rho_0] C_k \right] \rho^k = 0$$

$$\therefore \frac{C_{k+1}}{C_k} = \frac{2k+2l+2 - \rho_0}{(k+1)(k+2l+2)} \sim \frac{2}{k} \text{ as } k \rightarrow \infty$$

If ρ_0 is not an integer positive.

: This is a problem.

because $\frac{C_{k+1}}{C_k} \sim \Theta\left(\frac{1}{k}\right)$ gives $W(\rho) \sim \exp[\zeta\rho]$,

and then it changes the asymptotic behavior.

\Rightarrow Therefore, the term C_k has to be terminated at some power $k=N, s.t.$

$$\therefore \rho_0 = \boxed{\text{positive integer}} = 2(N+l+1) \equiv 2n$$

$$\Rightarrow E = -\frac{1}{2} \underbrace{mc^2}_{13.6 \text{ eV} \cdot Z^2} (Z\alpha)^2 \cdot \frac{1}{n^2} \quad || \quad n = \underbrace{\frac{N+l+1}{\text{---}}}_{= 1, 2, 3, 4 \dots}$$

$\rightarrow n = 1 \dots l = 0$ only allowed.

"principal quantum number"

$n = 2 \dots l = 0, 1$

$n = 3 \dots l = 0, 1, 2$

:

degeneracy of $E_n \leftarrow \# \text{ of } |n, l, m\rangle \text{ for a given } n.$

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$$= \sum_{l=0}^{n-1} 2l+1 = \underline{\underline{n^2}}$$

- The length scale κ in $\rho = \kappa r$ also n -dependent!

$$\frac{1}{\kappa} = \frac{\hbar}{m\alpha} \frac{n}{Z} \equiv a_0 \frac{n}{Z}$$

\rightarrow natural length scale $a_0 \equiv \frac{\hbar^2}{m\alpha} = \frac{\hbar^2}{me^2}$: Bohr radius

- finally, the wave function:

$$\psi_{nle}(\vec{r}) = R_{nle}(r) Y_e^m(\theta, \phi)$$

$$R_{nle}(r) = \left(\frac{Z}{na_0}\right)^l \cdot e^{-\frac{Zr}{na_0}} \sum_{k=0}^{\infty} C_k \left(\frac{Z}{na_0} r\right)^k$$

where $\frac{C_{k+1}}{C_k} = \frac{2(k+l+1-n)}{(k+1)(k+2l+2)}.$

- C_0 has to be determined by the normalization

$$\int_0^{\infty} r^2 dr |R_{nle}|^2 = 1.$$

- The other example in the S & N is the isotropic simple Harmonic Oscillator.

\leftarrow Try to solve it by yourself.

Caution: the asymptotic behavior at a large r is different.

* Implications of the degeneracy "n": Is it accidental?

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(S&N. ch.4.1)

for a given n , $l = 0, 1, \dots, n-1$ are allowed.

→ Maybe there exists some symmetry higher than $SO(3)$.

[$SO(3)$ indicates only $m = -l \dots l$ for a given l].

- In the Kepler problem in C.M. ($F(r) = -\frac{k_e}{r^2} \hat{r}$)

$\vec{A} = \vec{p} \times \vec{L} - m k_e \hat{r}$ is conserved.

: Laplace - Runge - Lenz or Runge - Lenz or Lenz vector.

→ The perihelion does not change in time.

- In Q.M., a Hermitian version of the Lenz vector :

$$\vec{M} = \frac{1}{2m} (\vec{p} \times \vec{L} - \vec{L} \times \vec{p}) - \frac{ze^2}{r} \vec{x} \quad \parallel \quad \text{For two Hermitian} \\ \vec{A}, \vec{B},$$

$$\Rightarrow \underline{[\vec{M}, H] = 0} \quad \text{for} \quad H = \frac{\vec{p}^2}{2m} - \frac{ze^2}{r} \quad (\vec{A} \times \vec{B})^+ = -\vec{B} \times \vec{A}$$

one can also find $\vec{L} \cdot \vec{M} = \vec{M} \cdot \vec{L} = 0$

$$\vec{M}^2 = \frac{1}{m} H (\vec{L}^2 + \vec{h}^2) + \vec{z}^2 e^4,$$

and

$$[L_i, L_j] = i\hbar \sum_{ijk} L_k$$

$$[M_i, M_j] = -i\hbar \sum_{ijk} \frac{2}{m} H L_k$$

$$[M_i, L_j] = i\hbar \sum_{ijk} M_k$$

This prevents us to make a closed algebra,

but, we can make it closed by considering energy eigenstates.

$$[L_i, L_j] = i\hbar \sum_{ijk} L_k$$

$$\Rightarrow H = E.$$

$$[N_i, N_j] = i\hbar \sum_{ijk} L_k$$

$$[N_i, L_j] = i\hbar \sum_{ijk} N_k.$$

$$\Leftrightarrow \vec{N} = \left(-\frac{m}{2E}\right)^{\frac{1}{2}} \vec{M}$$

6 generators of $SO(4)$. : rotations in 4D. 51

But, we can separate the algebra of $SO(4)$ into two sets of algebras.

If we define

$$\begin{bmatrix} \vec{I} = (\vec{L} + \vec{N})/2 \\ \vec{K} = (\vec{L} - \vec{N})/2 \end{bmatrix} \quad \begin{array}{l} \text{NOTE:} \\ [\vec{I}, H] = 0 \\ [\vec{K}, H] = 0 \end{array}$$

$$\Rightarrow [\vec{I}_i, \vec{I}_j] = i\hbar \epsilon_{ijk} I_k, \quad [\vec{K}_i, \vec{K}_j] = i\hbar \epsilon_{ijk} K_k, \quad [\vec{I}_i, \vec{K}_j] = 0$$

$\downarrow SU(2) \qquad \downarrow SU(2)$

$$\vec{I}^2 \rightarrow i(i+1) \hbar^2 \quad \text{if } i=0, \frac{1}{2}, 1, \frac{3}{2}, \dots \quad \vec{K}^2 \rightarrow k(k+1) \hbar^2 \quad \text{if } k=0, \frac{1}{2}, 1, \frac{3}{2}, \dots$$

$(2i+1) \text{ deg.} \qquad \qquad \qquad (2k+1) \text{ deg.}$

$$\text{Since } \vec{I}^2 - \vec{K}^2 = \vec{L} \cdot \vec{N} = 0, \quad k = i.$$

$$\text{The operator } \vec{I}^2 + \vec{K}^2 = \frac{1}{2} \left[\vec{L}^2 - \frac{m}{2E} \vec{M}^2 \right]$$

$$\text{goes to } 2k(k+1) \hbar^2 = \frac{1}{2} \left(-\hbar^2 - \frac{m}{2E} Z^2 e^4 \right)$$

$$\begin{array}{c} \swarrow \\ \vec{E} = -\frac{mZ^2 e^4}{2\hbar^2} \frac{1}{(2k+1)^2}, \quad k=0, \frac{1}{2}, 1, \frac{3}{2}, \dots \end{array} \quad \begin{array}{c} \downarrow \\ \vec{M}^2 = \frac{2}{m} H (\vec{L}^2 + \vec{K}^2) \\ + Z^2 e^4. \end{array}$$

$$= -\frac{mZ^2 e^4}{2\hbar^2} \frac{1}{n^2}, \quad n=1, 2, 3, 4, \dots$$

$$\therefore \text{deg.} = (2i+1) \cdot (2k+1) \Big|_{k=i} \quad \text{for a given } n.$$

$$= \boxed{n^2}$$

$$SO(4) = SU(2) \times SU(2)$$